



```

chain nodes :
  7 9 16 29 34 35 37 74
ring nodes :
  1 2 3 4 5 6 10 11 12 13 14 15 17 18 19 20 21 22 23 24 25 26 27 28 38
  39 40 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66
  67 68
chain bonds :
  1-34 4-35 7-9 7-14 16-21 27-29 35-37 37-74
ring bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 5-38 6-40 10-11 10-15 11-12 12-13 13-14 14-15 17-18
  17-22 18-19 19-20 20-21 21-22 23-24 23-28 24-25 25-26 26-27 27-28 38-39 39-40
  45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 55-56 57-58
  57-62 58-59 59-60 60-61 61-62 63-64 63-68 64-65 65-66 66-67 67-68
exact/norm bonds :
  1-34 4-35 5-38 6-40 7-9 7-14 10-11 10-15 11-12 12-13 13-14 14-15 16-21 17-18
  17-22 18-19 19-20 20-21 21-22 23-24 23-28 24-25 25-26 26-27 27-28 27-29 35-37
  37-74 38-39 39-40
normalized bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53
  53-54 54-55 55-56 57-58 57-62 58-59 59-60 60-61 61-62 63-64 63-68 64-65 65-66
  66-67 67-68

```

```

G2:O,S,N
G3:[*1],[*2],[*3]
G4:C,S,N
G5:C,N
G6:Cb,[*4],[*5],[*6],[*7]

```

```

Match level :
  1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom
  13:Atom

```

	14:Atom	15:Atom	16:CLASS	17:Atom	18:Atom	19:Atom	20:Atom	21:Atom	22:Atom
23:Atom	24:Atom	25:Atom	26:Atom	27:Atom	28:Atom	29:CLASS	34:CLASS	35:CLASS	37:CLASS
38:Atom	39:Atom	40:Atom	45:Atom	46:Atom	47:Atom	48:Atom	49:Atom	50:Atom	51:Atom
52:Atom	53:Atom	54:Atom	55:Atom	56:Atom	57:Atom	58:Atom	59:Atom	60:Atom	61:Atom
62:Atom	63:Atom	64:Atom	65:Atom	66:Atom	67:Atom	68:Atom	74:CLASS		